

CHEMISTRY 606
Fall 2002
10:00-10:50 a.m. MWF
331 Lloyd Hall

X-RAY CRYSTALLOGRAPHY

Dr. R. D. ROGERS
OFFICE: 126A Lloyd Hall
OFFICE HOURS: By Appt.

TEXTS: 1) G. H. Stout and L. H. Jensen, *X-ray Structure Determination. A Practical Guide*; 2nd ed., Wiley, 1989; 2) IUCr Commission on Crystallographic Teaching: Booklets 1-19.

SUPPLEMENTAL TEXTS: At times during the semester we may also refer to the following books: 1) J. P. Glusker and K. N. Trueblood, *Crystal Structure Analysis, A Primer*, 2nd ed., Oxford, 1985; 2) C. Hammond, *Introduction to Crystallography*, Revised ed., Oxford, 1992; 3) D. Sherwood, *Crystals, X-rays and Proteins*, Wiley, 1976; d) Class Handouts.

COURSE OVERVIEW: This will be a workshop-based course with the emphasis on *work*. The course will include: a) lectures when appropriate, b) reading assignments, c) problems (book and computer) assignments, d) classroom discussion, e) student led discussion and presentations, f) hands-on work with the diffractometer and computer systems, g) critical evaluation of the crystallographic literature, and h) writing a paper for publication. Each student will be expected to participate fully in all activities.

If you have a crystal you would like to study you may use it, otherwise one will be provided for you. (If you use your own crystal, you must get permission to publish the results at the end of the course!) By the end of the semester you will have selected an appropriate crystal, collected the data, solved the structure, and submitted a paper for publication based on the results.

Each student will be given many assignments to present to the class or to lead discussion. If time permits, students will be allowed to introduce new topics for class discussion. It is strongly recommended that each student keep two notebooks: one for theory and class notes, a second one for all explicit techniques and operations. The second reference notebook can then be used after the course for a general outline of procedures.

Each student will need access to a computer (PC not Mac); preferably their own and preferably a laptop. If you do not have access to a computer, please make arrangements as soon as possible to get access. It will be necessary to load software on this computer.

GRADING: Final grades will be determined by class participation (15%), problem assignments (20%), a paper written for publication (20%), a midterm exam (20%), and a comprehensive final exam (25%).

GENERAL TOPICS TO BE COVERED:

1. Crystals and Symmetry
2. X-rays and Diffraction
3. Data Collection
4. Data Reduction and Theory
5. The Phase Problem
6. Patterson Methods/Direct Methods in Structure Solution
7. Structure Refinement Strategies
8. Structure Interpretation
9. Interpretation of the Crystallographic Literature
10. Hot Topics in Solid State Science
11. Publication of Crystallographic Data

SPECIAL DATES:

August 21: First Day of Class
September 2: No Class (Labor Day)
November 29: No Class (Thanksgiving)
December 6: Last Class Day
December 12: Final Exam (11:30 am-2:00 pm)

Disability access statement: "To request disability accommodations, please contact the Office of Disability Services at 348-4285. After initial arrangements are made with that office, contact your professor."